

## Connecting via Winsock to STN

10/784,9168.

3(3/01)

# Structure search of elelctro comp

Welcome to STN International! Enter x:x

LOGINID: SSSPTAAJP1626

**PASSWORD:**

TERMINAL (ENTER 1, 2, 3, OR ?):2

\* \* \* \* \* \* \* \* \* \* \* \* \* \* \* Welcome to STN International \* \* \* \* \* \* \* \* \* \* \*

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America  
NEWS 2 "Ask CAS" for self-help around the clock  
NEWS 3 SEP 01 New pricing for the Save Answers for SciFinder Wizard within STN Express with Discover!  
NEWS 4 OCT 28 KOREAPAT now available on STN  
NEWS 5 NOV 30 PHAR reloaded with additional data  
NEWS 6 DEC 01 LISA now available on STN  
NEWS 7 DEC 09 12 databases to be removed from STN on December 31, 2004  
NEWS 8 DEC 15 MEDLINE update schedule for December 2004  
NEWS 9 DEC 17 ELCOM reloaded; updating to resume; current-awareness alerts (SDIs) affected  
NEWS 10 DEC 17 COMPUAB reloaded; updating to resume; current-awareness alerts (SDIs) affected  
NEWS 11 DEC 17 SOLIDSTATE reloaded; updating to resume; current-awareness alerts (SDIs) affected  
NEWS 12 DEC 17 CERAB reloaded; updating to resume; current-awareness alerts (SDIs) affected  
NEWS 13 DEC 17 THREE NEW FIELDS ADDED TO IFIPAT/IFIUDB/IFICDB  
NEWS 14 DEC 30 EPFULL: New patent full text database to be available on STN  
NEWS 15 DEC 30 CAPLUS - PATENT COVERAGE EXPANDED  
NEWS 16 JAN 03 No connect-hour charges in EPFULL during January and February 2005  
NEWS 17 FEB 25 CA/CAPLUS - Russian Agency for Patents and Trademarks (ROSPATENT) added to list of core patent offices covered  
NEWS 18 FEB 10 STN Patent Forums to be held in March 2005  
NEWS 19 FEB 16 STN User Update to be held in conjunction with the 229th ACS National Meeting on March 13, 2005  
NEWS 20 FEB 28 PATDPAFULL - New display fields provide for legal status data from INPADOC  
NEWS 21 FEB 28 BABS - Current-awareness alerts (SDIs) available  
NEWS 22 FEB 28 MEDLINE/LMEDLINE reloaded  
NEWS 23 MAR 02 GBFULL: New full-text patent database on STN  
NEWS 24 MAR 03 REGISTRY/ZREGISTRY - Sequence annotations enhanced  
  
NEWS EXPRESS JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005  
  
NEWS HOURS STN Operating Hours Plus Help Desk Availability  
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\* \*

FILE 'HOME' ENTERED AT 14:20:05 ON 03 MAR 2005

=> fil reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

FULL ESTIMATED COST

ENTRY

0.21

SESSION

0.21

FILE 'REGISTRY' ENTERED AT 14:20:15 ON 03 MAR 2005

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 2 MAR 2005 HIGHEST RN 841200-41-7

DICTIONARY FILE UPDATES: 2 MAR 2005 HIGHEST RN 841200-41-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

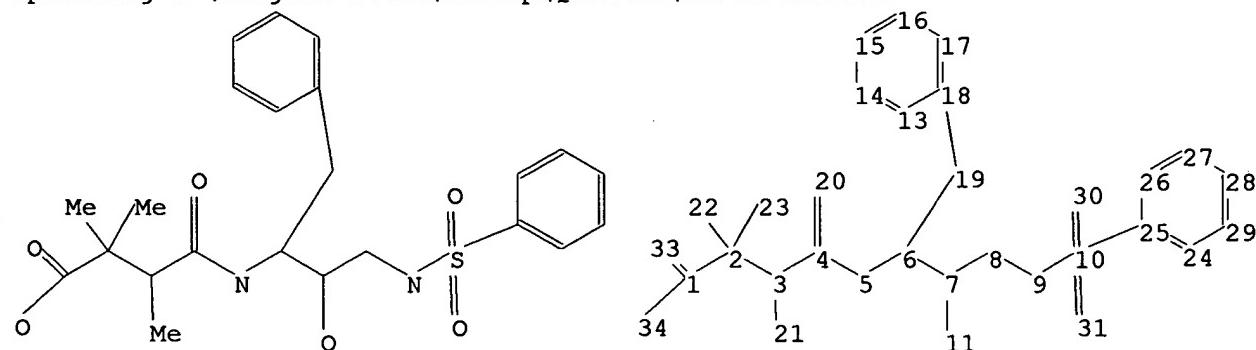
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

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Uploading C:\Program Files\Stnexp\Queries\10784916b.str



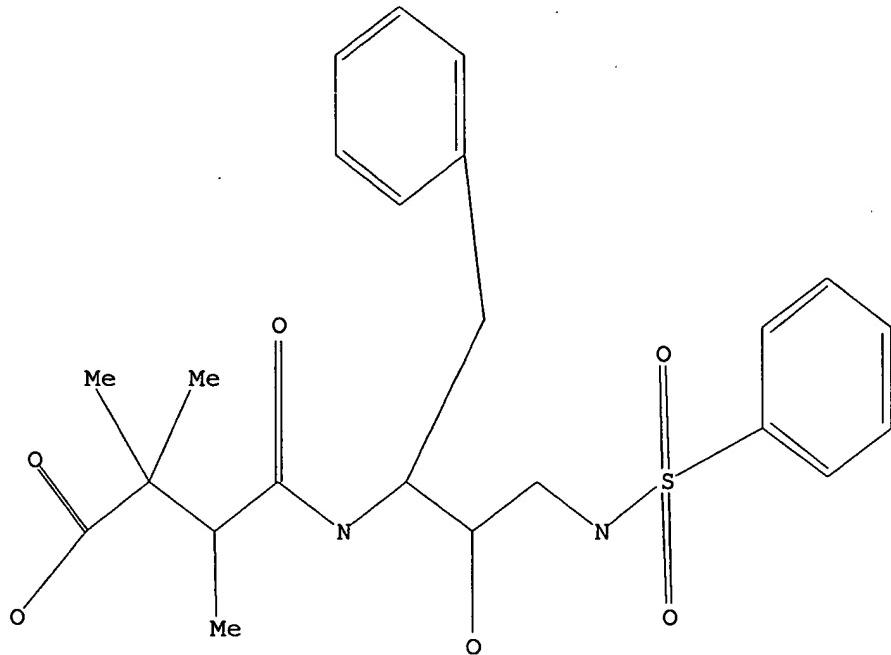
chain nodes :

1 2 3 4 5 6 7 8 9 10 11 19 20 21 22 23 30 31 33 34  
 ring nodes :  
 13 14 15 16 17 18 24 25 26 27 28 29  
 chain bonds :  
 1-2 1-33 1-34 2-3 2-22 2-23 3-4 3-21 4-5 4-20 5-6 6-7 6-19 7-8 7-11  
 8-9 9-10 10-30 10-31 10-25 18-19  
 ring bonds :  
 13-14 13-18 14-15 15-16 16-17 17-18 24-25 24-29 25-26 26-27 27-28 28-29  
 exact/norm bonds :  
 4-5 4-20 5-6 7-11 8-9 9-10 10-30 10-31 10-25  
 exact bonds :  
 1-2 2-3 2-22 2-23 3-4 3-21 6-7 6-19 7-8 18-19  
 normalized bonds :  
 1-33 1-34 13-14 13-18 14-15 15-16 16-17 17-18 24-25 24-29 25-26 26-27  
 27-28 28-29

Hydrogen count :  
 11:= exact 1 34:= exact 1  
 Connectivity :  
 9:3 M minimum RC ring/chain  
 Match level :  
 1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS  
 10:CLASS 11:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS  
 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom  
 29:Atom 30:CLASS 31:CLASS 33:CLASS 34:CLASS

L1 STRUCTURE UPLOADED

=> d  
 L1 HAS NO ANSWERS  
 L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s L1  
SAMPLE SEARCH INITIATED 14:20:43 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 46 TO ITERATE

100.0% PROCESSED 46 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 514 TO 1326  
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s L1 full  
FULL SEARCH INITIATED 14:20:47 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 877 TO ITERATE

100.0% PROCESSED 877 ITERATIONS 5 ANSWERS  
SEARCH TIME: 00.00.01

L3 5 SEA SSS FUL L1

=> fil caplus  
COST IN U.S. DOLLARS SINCE FILE TOTAL  
ENTRY SESSION  
FULL ESTIMATED COST 161.33 161.54

FILE 'CAPLUS' ENTERED AT 14:20:54 ON 03 MAR 2005  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
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FILE COVERS 1907 - 3 Mar 2005 VOL 142 ISS 10  
FILE LAST UPDATED: 2 Mar 2005 (20050302/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s L3

L4 3 L3

=> d L4 ibib abs hitstr 1-3

L4 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 1996:47171 CAPLUS

DOCUMENT NUMBER: 124:193129

TITLE: Determination of protein binding by in vitro charcoal adsorption

AUTHOR(S): Yuan, Jinhua; Yang, Dai Chang; Birkmeier, Jill;

has exact elected  
SPP  
Final  
assigned  
for date

CORPORATE SOURCE:

Stolzenbach, James  
Pharmacokinetics, Bioanalytical and Radiochemistry  
Function, G. D. Searle Research and Development,  
Skokie, IL, 60077, USA

SOURCE:

Journal of Pharmacokinetics and Biopharmaceutics  
(1995), 23(1), 41-55  
CODEN: JPBPB; ISSN: 0090-466X

PUBLISHER:

Plenum

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB Certain compds. such as SC-52151 have extensive nonspecific adsorption to the ultrafiltration devices or to dialysis membranes and therefore can not be measured by the conventional ultrafiltration or equilibrium dialysis methods. A new method based on charcoal adsorption was developed to overcome this difficulty. Unlike many conventional methods, which are based on the separation of free drug from bound drug under equilibrium conditions,

the new method is operated under nonequil. conditions and involves measuring the time course of decline of the percentage of bound drug remaining in plasma while the free drug is being removed by charcoal adsorption. Theor. aspects of the method and the data processing procedure are presented. SC-98A, a compound with minimal nonspecific adsorption to the ultrafiltration membrane, was used to demonstrate the applicability of this method against the ultrafiltration method. Using this method, the protein binding of SC-52151 in human plasma at 1.0 µg/mL was determined to be in the range of 91.4-97.7% at room temperature

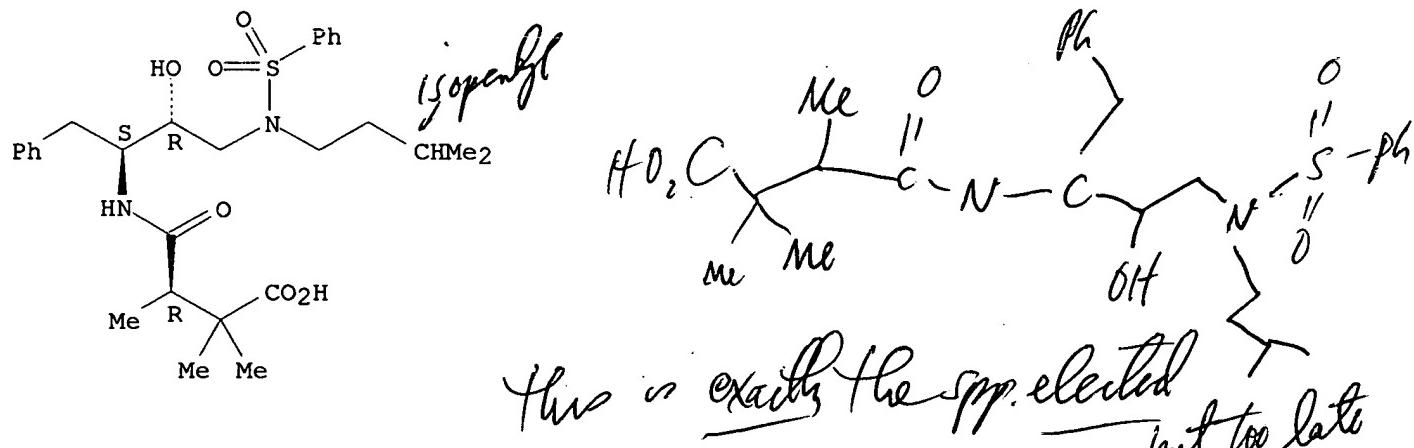
IT 157445-98-2, SC 98A

RL: BPR (Biological process); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses) (protein binding determination by in vitro charcoal adsorption)

RN 157445-98-2 CAPLUS

CN Butanoic acid, 4-[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1995:964989 CAPLUS

DOCUMENT NUMBER: 124:176937

TITLE: N-[(Succinoylamino)hydroxypropyl]sulfonamides useful as retroviral protease inhibitors

INVENTOR(S): Vazquez, Michael L.; Mueller, Richard A.; Talley, John J.; Getman, Daniel; Decrescenzo, Gary A.; Freskos, John N.

PATENT ASSIGNEE(S): G. D. Searle and Co., USA

SOURCE: U.S., 32 pp. Cont.-in-part of U.S. Ser. No. 935,490,

DOCUMENT TYPE:  
LANGUAGE:  
FAMILY ACC. NUM. COUNT: 2  
PATENT INFORMATION:

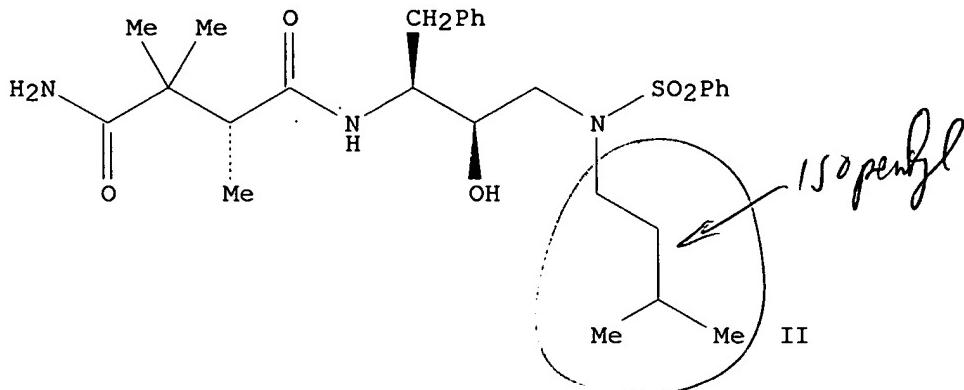
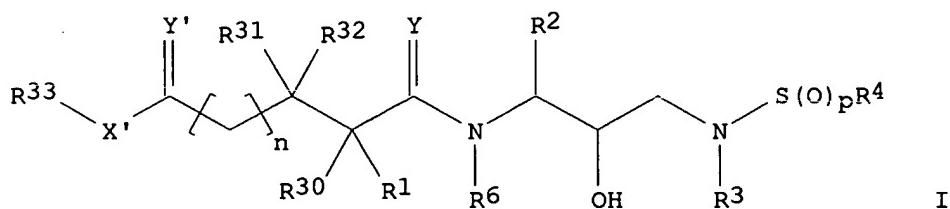
abandoned  
CODEN: USXXAM

*our app line*

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5463104	A	19951031	US 1993-110912	19930824
AT 154800	E	19970715	AT 1993-920213	19930824
ES 2103488	T3	19970916	ES 1993-920213	19930824
US 5714605	A	19980203	US 1995-541350	19951010
US 5760076	A	19980602	US 1995-541747	19951010
US 6022994	A	20000208	US 1998-41016	19980312
US 6313345	B1	20011106	US 1999-419816	19991018
US 2002137942	A1	20020926	US 2001-884462	20010620
US 6469207	B2	20021022		
US 2003220508	A1	20031127	US 2002-237184	20020909
US 6727282	B2	20040427		
US 2005004043	A1	20050106	US 2004-784916	20040224
<i>Priority Appln. Info.:</i>				
			US 1992-935490	B2 19920825
			US 1993-110912	A3 19930824
			US 1995-541350	A1 19951010
			US 1995-541747	A1 19951010
			US 1998-41016	A1 19980312
			US 1999-419816	A1 19991018
			US 2001-884462	A1 20010620
			US 2002-237184	A1 20020909

OTHER SOURCE(S):  
GI

MARPAT 124:176937



AB Succinoylamino hydroxyethylamino sulfonamide compds. I or a pharmaceutically acceptable salt or ester thereof, wherein p represents 0,

1 or 2; n represents either 0 or 1; X' represents N(R34) or O; or R33X' represents cycloalkyl or aryl radicals; Y and Y' each independently represent O or S; R1, R30, R31 and R32 each independently represent hydrogen, OH, (CH<sub>2</sub>)C(O)CH<sub>3</sub>, CH<sub>2</sub>SO<sub>2</sub>NH<sub>2</sub>, CO<sub>2</sub>CH<sub>3</sub>, CONHCH<sub>3</sub>, CON(CH<sub>3</sub>)<sub>2</sub>, CH<sub>2</sub>C(O)NHCH<sub>3</sub>, CH<sub>2</sub>C(O)N(CH<sub>3</sub>)<sub>2</sub>, CONH<sub>2</sub>, C(CH<sub>3</sub>)<sub>2</sub>(SH), C(CH<sub>3</sub>)<sub>2</sub>(SCH<sub>3</sub>), C(CH<sub>3</sub>)<sub>2</sub>[S(O)CH<sub>3</sub>], C(CH<sub>3</sub>)<sub>2</sub>[S(O)CH<sub>3</sub>], alkyl, haloalkyl, alkenyl, alkynyl, aralkyl or cycloalkyl radicals, or the side chain of the amino acid asparagine, S-Me cysteine or the corresponding sulfoxide or sulfone derivs. thereof, leucine, isoleucine, allo-isoleucine, tert-leucine, phenylalanine, ornithine, alanine, norleucine, glutamine, valine, threonine, serine, o-alkyl serine, aspartic acid, β-cyanoalanine or allo-threonine; or R30 and R32 together with the carbon atoms to which they are attached form a cycloalkyl radical; R2 = e.g., alkyl, aryl, cycloalkyl; R3, R33, R34 = e.g., H, alkyl, haloalkyl; R4 = e.g., alkyl, haloalkyl, alkenyl; R6 = H, alkyl; are effective as retroviral protease inhibitors, and in particular as inhibitors of HIV protease. Thus, e.g., butanediamide II was prepared by coupling of benzyl (R)-2,2,3-trimethylsuccinate (preparation given) with 2(R)-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1(S)-(phenylmethyl)propylamine (preparation given) followed by benzyl ester hydrogenolysis and amidation, and exhibited IC<sub>50</sub> = 2 nM for inhibition of HIV protease.

IT 157445-98-2P 157446-00-9P 157446-03-2P  
157446-09-8P 157474-44-7P

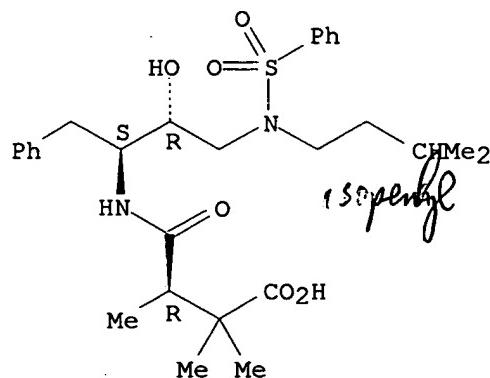
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(N-[(succinoylamino)hydroxypropyl]sulfonamides useful as retroviral protease inhibitors)

RN 157445-98-2 CAPLUS

CN Butanoic acid, 4-[[[1S,2R]-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, (3R)- (9CI) (CA INDEX NAME)

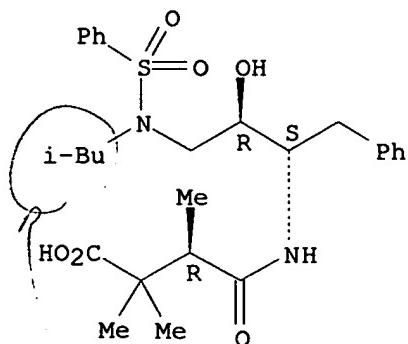
Absolute stereochemistry.



RN 157446-00-9 CAPLUS

CN Butanoic acid, 4-[[2-hydroxy-3-[(2-methylpropyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, [1S-[1R\*(S\*),2S\*]]- (9CI) (CA INDEX NAME)

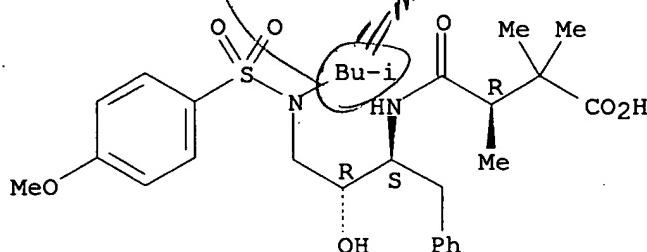
Absolute stereochemistry.



RN 157446-03-2 CAPLUS

CN Butanoic acid, 4-[[2-hydroxy-3-[(4-methoxyphenyl)sulfonyl](2-methylpropyl)amino]-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-[1S-[1R\*(S\*),2S\*]]- (9CI) (CA INDEX NAME)

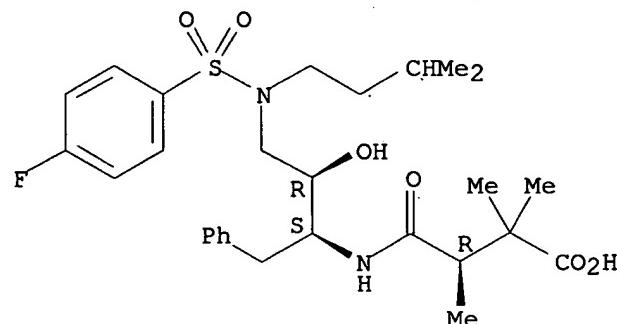
Absolute stereochemistry.



RN 157446-09-8 CAPLUS

CN Butanoic acid, 4-[[3-[(4-fluorophenyl)sulfonyl](3-methylbutyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-[1S-[1R\*(S\*),2S\*]]- (9CI) (CA INDEX NAME)

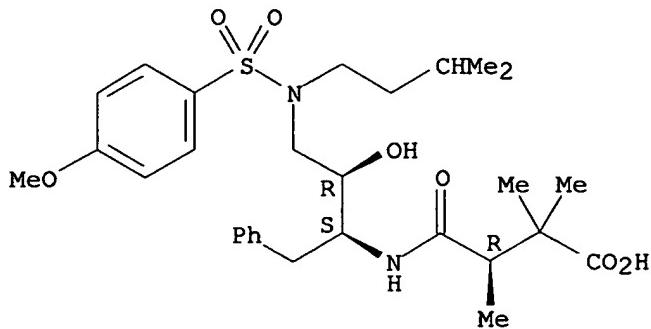
Absolute stereochemistry.



RN 157474-44-7 CAPLUS

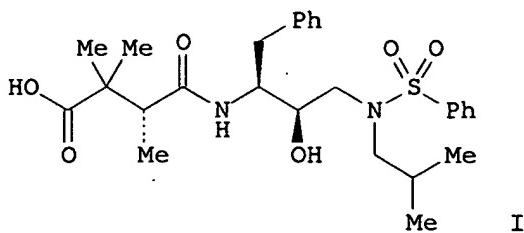
CN Butanoic acid, 4-[[2-hydroxy-3-[(4-methoxyphenyl)sulfonyl](3-methylbutyl)amino]-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-[1S-[1R\*(S\*),2S\*]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1994:579258 CAPLUS  
 DOCUMENT NUMBER: 121:179258  
 TITLE: N-(alkanoylamino-2-hydroxypropyl)sulfonamides useful as HIV protease inhibitors  
 INVENTOR(S): Vazquez, Michael L.; Mueller, Richard A.; Talley, John J.; Getman, Daniel; Decrescenzo, Gary A.; Freskos, John N.  
 PATENT ASSIGNEE(S): G.D. Searle and Co., USA; Monsanto Co.  
 SOURCE: PCT Int. Appl., 103 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9404491	A1	19940303	WO 1993-US7815	19930825
W: AT, AU, BB, BG, BR, BY, CA, CH, CZ, DE, DK, ES, FI, GB, HU, JP, KP, KR, KZ, LK, LU, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SK, UA, US, VN				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
EP 656886	A1	19950614	EP 1993-920213	19930824
EP 656886	B1	19970625		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
JP 08500824	T2	19960130	JP 1993-506531	19930824
AT 154800	E	19970715	AT 1993-920213	19930824
ES 2103488	T3	19970916	ES 1993-920213	19930824
AU 674702	B2	19970109	AU 1993-50819	19930825
AU 9350819	A1	19940315		
RU 2130016	C1	19990510	RU 1995-106823	19930825
NO 9500670	A	19950222	NO 1995-670	19950222
FI 9500841	A	19950223	FI 1995-841	19950223
PRIORITY APPLN. INFO.:			US 1992-935490	A2 19920825
			WO 1993-US7815	W 19930825
OTHER SOURCE(S): GI	MARPAT	121:179258		



I

AB The title compds. R<sub>33</sub>(R<sub>34</sub>)X<sub>1</sub>C(:Y<sub>1</sub>)(CH<sub>2</sub>)TC(R<sub>31</sub>)(R<sub>32</sub>)C(R<sub>30</sub>)(R<sub>1</sub>)C(:Y)N(R<sub>6</sub>)C(R<sub>2</sub>)HC(OH)HCH<sub>2</sub>N(R<sub>3</sub>)S(O)xR<sub>4</sub> [R<sub>1</sub> = H, CH<sub>2</sub>SO<sub>2</sub>NH<sub>2</sub>, CO<sub>2</sub>Me, CONHMe, CONMe<sub>2</sub>, etc.; R<sub>2</sub> = alkyl, aryl, cycloalkyl, (un)substituted cycloalkylalkyl and arylalkyl; R<sub>3</sub> = H, alkyl, haloalkyl, alkenyl, alkynyl, hydroxyalkyl, alkoxyalkyl, cycloalkyl, etc.; R<sub>4</sub> = alkyl, haloalkyl alkenyl, alkynyl, hydroxyalkyl, alkoxyalkyl, cycloalkyl etc.; R<sub>6</sub> = H, alkyl; R<sub>30</sub>-R<sub>32</sub> = R<sub>1</sub>; R<sub>1</sub>R<sub>30</sub>R<sub>31</sub> = cycloalkyl; R<sub>1</sub>R<sub>30</sub>R<sub>32</sub>C = cycloalkyl; R<sub>33</sub>, R<sub>34</sub> = H, R<sub>3</sub>; R<sub>33</sub>R<sub>34</sub>X<sub>1</sub> = cycloalkyl, aryl, heterocyclyl, etc.; X<sub>1</sub> = O, N, CR<sub>17</sub>; R<sub>17</sub> = H, alkyl; Y, Y<sub>1</sub> = O, S, NR<sub>15</sub>; R<sub>15</sub> = H, R<sub>3</sub>; t = 0, 1; x = 0-2], useful as HIV protease inhibitors for the treatment of AIDS, are prepared. Thus, sulfonamide I was prepared and demonstrated IC<sub>50</sub> against HIV protease of 1 nmol.

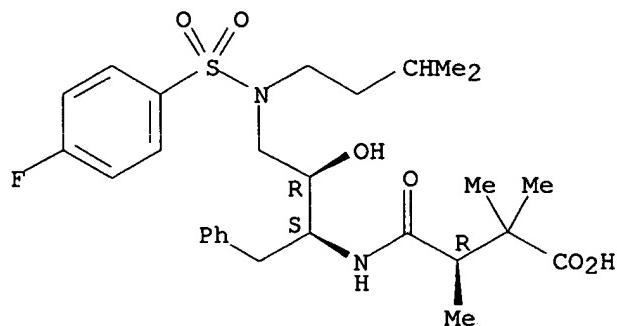
IT 157446-09-8 157474-44-7

RL: RCT (Reactant); RACT (Reactant or reagent)  
(HIV protease inhibitor)

RN 157446-09-8 CAPLUS

CN Butanoic acid, 4-[[3-[(4-fluorophenyl)sulfonyl](3-methylbutyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, [1S-[1R\*(S\*),2S\*]]- (9CI) (CA INDEX NAME)

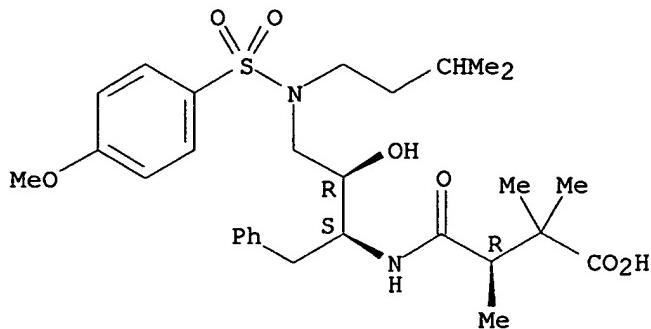
Absolute stereochemistry.



RN 157474-44-7 CAPLUS

CN Butanoic acid, 4-[[2-hydroxy-3-[(4-methoxyphenyl)sulfonyl](3-methylbutyl)amino]-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, [1S-[1R\*(S\*),2S\*]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



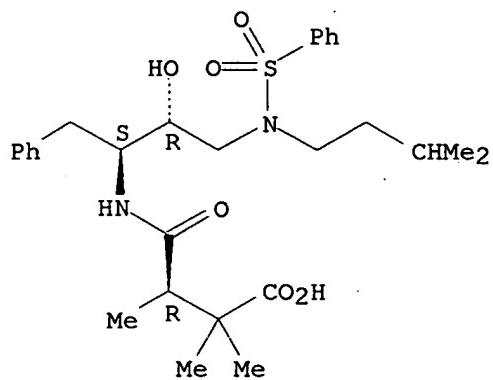
IT 157445-98-2P 157446-00-9P 157446-03-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of, as HIV protease inhibitor)

RN 157445-98-2 CAPLUS

CN Butanoic acid, 4-[[1S,2R]-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, (3R)- (9CI) (CA INDEX NAME)

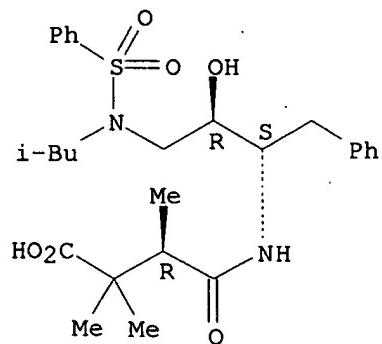
Absolute stereochemistry.



RN 157446-00-9 CAPLUS

CN Butanoic acid, 4-[[2-hydroxy-3-[(2-methylpropyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, [1S-[1R\*(S\*),2S\*]]- (9CI) (CA INDEX NAME)

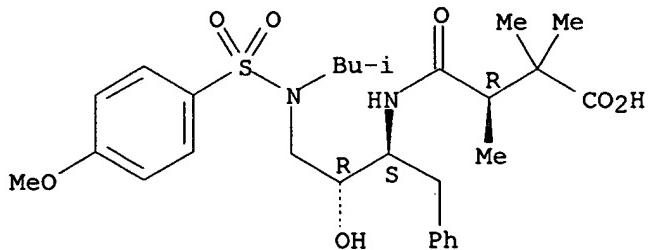
Absolute stereochemistry.



RN 157446-03-2 CAPLUS

CN Butanoic acid, 4-[[2-hydroxy-3-[(4-methoxyphenyl)sulfonyl](2-methylpropyl)amino]-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, [1S-[1R\*(S\*),2S\*]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> FIL STNGUIDE

COST IN U.S. DOLLARS

SINCE FILE

ENTRY

TOTAL

SESSION